Pathology of Schwinger boson mean field theory for Heisenberg spin models

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Abstract

We re-analyze the Schwinger boson mean field theory (SBMFT) for Heisenberg spin models on the cubic lattice. We find that the second order phase transition point for magnetic ordering previously reported corresponds to a local maximum of the free energy functional. For both ferromagnetic and antiferromagnetic Heisenberg models with spin $S \geq S_C$, where $S_C < 1/2$, the mean field transitions are first order from the magnetically long-ranged ordered phase to the completely uncorrelated phase. In addition to erroneously giving a first order transition for magnetic ordering, the mean field theory does not include a phase with finite short-range correlation, thus negating one of the prime advantages of SBMFT. The relevance of these pathologies to other situations beyond the cubic lattice is discussed.

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I. INTRODUCTION

Schwinger boson representation is by now a well known tool in the study of quantum spin systems [1–3]. In this method, each spin operator is represented by two Schwinger bosons. In contrast to Holstein-Primakoff bosons [4], the Schwinger boson representation of spin operators does not involve square roots. Furthermore, while the vacuum state of Holstein-Primakoff bosons has to be a broken symmetry state, this is not the case for Schwinger bosons. Instead, long-ranged order (LRO) is a result of condensation of the Schwinger bosons [2,3]. Thus, using Schwinger bosons allows one to naturally address both the magnetically disordered and ordered states.

Using the Schwinger boson representation, the quantum spin Hamiltonian is mapped onto an interacting boson Hamiltonian, which can then be approximated by a self-consistent non-interacting Hamiltonian using mean field theory (MFT). In such a mean field theory, a non-zero mean field amplitude corresponds to short-ranged order (SRO). Long range order exists only if for a given temperature, the mean field Hamiltonian gives rise to Bose condensation. The ability of the mean field theory to address both short-ranged and long-ranged order is perhaps its most appealing feature, especially for 1D and 2D systems, where exact solutions has shown that LRO is destroyed at any finite temperature. For the Heisenberg ferromagnetic or antiferromagnetic Hamiltonian on a d-dimensional hypercubic lattice, the results reported in literature are briefly summarized as follows. In both 1D and 2D, in agreement with exact results, there is no LRO at any finite temperature. However, SRO persists until a certain temperature is exceeded [1–3]. In 3D, LRO is stable at low temperature, and there is a continuous phase transition into the SRO state at some critical temperature. Within Schwinger boson MFT (SBMFT), the order-disorder transition has the usual mean field exponents [2].

In this paper, we re-examine the SBMFT for the Heisenberg spin Hamiltonian on the 3D cubic lattice. We find that, provided the spin S is greater than some critical value S_c ($< 1/2$), the previously reported mean field solution that exhibits a continuous phase transition for

magnetic LRO is actually an unstable solution corresponding to a local *maximum* of the free energy. Instead, the minimum free energy solution shows a first order transition. Since it is well established that the Heisenberg Hamiltonian has a continuous transition in 3D, our analysis raises serious question about the applicability of the SBMFT in 3D. Furthermore, the first order transition is into a state with zero mean field amplitude, i.e., without any correlation. Thus, the supposed advantage of SBMFT of being able to describe SRO does not actually exist. These pathologies of the SBMFT are not restricted to 3D, but should appear whenever the LRO can be destroyed by tuning some parameter. An example of which is the bilayered Heisenberg antiferromagnet at $T = 0$ where as the inter-layer coupling is increased, SBMFT also shows a first order transition into the uncorrelated state [5].

The rest of this paper is organized as follows. In Section II and III, we will discuss the SBMFT solutions for the Heisenberg ferromagnet and antiferromagnet separately, showing that the same pathologies are seen in both cases. These results will be summarized in Section IV, where we will also discuss their relevance to the bilayered Heisenberg antiferromagnet.

II. FERROMAGNETIC HEISENBERG MODEL

In this section we discuss the SBMFT for the FM Heisenberg model. We first briefly review the Schwinger boson representation and its mean field equations [1–3]. We then discuss the mean field solutions of the model with emphasis on 3D.

We study a spin-S Heisenberg ferromagnet in a d-dimensional hypercubic lattice with periodic boundary conditions,

$$H = -J \sum_{<i,j>} S_i \cdot S_j, \tag{1}$$

where the exchange constant $J > 0$ and the sum is over all the nearest-neighbor pairs on the lattice. In the Schwinger boson representation, a spin operator is represented by two types of bosons,

$$S_i^z = \frac{1}{2}(a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow}), \tag{2}$$

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$$S_i^+ = a_{i\uparrow}^\dagger a_{i\downarrow}, \ S_i^- = a_{i\downarrow}^\dagger a_{i\uparrow}, \tag{3}$$

These bosons should satisfy the constraints in their Fock space as follows, $\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} = 2S$, with $2S = 1$, 2, ... for physical systems. By introducing a bond operator, $B_{ij}^\dagger = \frac{1}{2}\sum_\sigma a_{i\sigma}^\dagger a_{j\sigma}$, the SU(2) FM Heisenberg Hamiltonian can be written as,

$$H_{FM-B} = -2J \sum_{<ij>} : B_{ij}^\dagger B_{ij} : + \frac{NzJ}{2}S^2 + \sum_i \lambda_i (\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} - 2S). \tag{4}$$

In the above Eqn., $::$ denotes a normal ordering of the bosonic operators, N is the number of sites in the lattice, and $z = 2\,d$ is the nearest neighbor coordinate. A Lagrangian multiplier field λ_i for the constraint on site i is introduced. Note that the FM Heisenberg model is now transformed to an interacting boson model.

To proceed further, a bond mean field amplitude $B = < B_{ij}^+ > = < B_{ij} >$, assumed to be real and uniform, is introduced. Neglecting fluctuations, the following non-interacting mean field Hamiltonian is obtained.,

$$H_{MF} = \lambda \sum_i (\sum_\sigma a_{i\sigma}^\dagger a_{i\sigma} - 2S) - 2J \sum_{ij} B(B_{ij}^\dagger + B_{ij}) + \frac{NzJ}{2}S^2 + NzJB^2, \tag{5}$$

In H_{MF} the local constraint at every site is replaced by a global one, and a non-zero value of B indicates *short-range* spin-spin correlation. The mean field Hamiltonian can be diagonalized, and we obtain

$$H_{MF} = \frac{NzJ}{2}S^2 + NzJB^2 - 2S\lambda N + \sum_{\vec{k},\sigma} \omega_{\vec{k}} a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma}, \tag{6}$$

where the energy dispersion is given by $\omega_{\vec{k}} = JzB(\epsilon_{\vec{k}} + \Lambda)$, with $\epsilon_{\vec{k}} = \frac{1}{z}\sum_{\vec{\delta}}(1 - e^{i\vec{k}.\vec{\delta}})$, and $\Lambda = \frac{\lambda}{JBz} - 1$.

The free energy per site is then given by

$$f = \frac{JS^2 z}{2} + zJB^2 - 2S\lambda - \frac{2}{\beta N}\sum_{\vec{k}} \log(\frac{1}{1 - e^{-\beta\omega_{\vec{k}}}}), \tag{7}$$

where $\beta = \frac{1}{k_B T}$, with k_B the Boltzmann constant and T the temperature. The amplitudes of the mean fields B and λ are obtained by minimizing the free energy, which leads to two coupled mean field eqns.,

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$$S = \frac{1}{N} \sum_{\vec{k}} \frac{1}{e^{\tilde{\beta}(\epsilon_{\vec{k}}+\Lambda)} - 1}, \tag{8}$$

$$B^2 = \frac{B}{N} \sum_{\vec{k}} \frac{1 - \epsilon_{\vec{k}}}{e^{\tilde{\beta}(\epsilon_{\vec{k}}+\Lambda)} - 1}, \tag{9}$$

where $\tilde{\beta} = 1/k_B \tilde{T}$, and $\tilde{T} = T/(JzB)$ acts as an effective temperature. In these eqns., $-\Lambda$ may be viewed as an effective chemical potential. Since $\epsilon_{\vec{k}} \geq 0$, we have $\Lambda \geq 0$. Magnetic long range order corresponds to Schwinger boson condensation at $\vec{k} = 0$ [2,3]. Since bosons do not condense at finite temperature in 1D or 2D, the 1D model and the 2D model are disordered at any temperature. In three and higher dimensions, one expects a finite critical temperature T_C, below which SBMFT gives a magnetic ordered state.

To study the possible magnetically ordered phase, the Schwinger boson condensate density $\rho = < a^{\dagger}_{\vec{k}=0,\sigma} a_{\vec{k}=0,\sigma} > /N$ is introduced, and the coupled mean field eqns. are rewritten as,

$$S = \rho + \int \frac{d^d \vec{k}}{(2\pi)^d} \frac{1}{e^{\tilde{\beta}(\epsilon_{\vec{k}}+\Lambda)} - 1}, \tag{10}$$

$$B^2 = B(S - \int \frac{d^d \vec{k}}{(2\pi)^d} \frac{\epsilon_{\vec{k}}}{e^{\tilde{\beta}(\epsilon_{\vec{k}}+\Lambda)} - 1}). \tag{11}$$

In the Bose condensed state, $\rho > 0$, $\Lambda = 0$, and $B \neq 0$; In the disordered state, $\rho = 0$, and $\Lambda > 0$. Sarker et al. [2] determined the critical temperature by requiring $\Lambda = 0$ and $\rho = 0$. This transition point will be labeled as "a", with the effective temperature $\tilde{T}_a$. By expanding equations 10 and 11 about $\tilde{T}_a$, the transition was determined to be continuous with mean field exponents. Upon re-examination of the mean field equations, we have, however, found the transition point $\tilde{T}_a$ to be physically inaccessible if the spin S is greater than some S_C. To understand this, we note that these equations are well-behaved in term of $\tilde{T}$. For example, the quantity B is smooth and monotomically decreasing as $\tilde{T}$ increases as one would expect. This is shown in fig. 1 for the case of $S = 1/2$. At $\tilde{T} = 0$, B is finite, and $\Lambda = 0$. As $\tilde{T}$ increases, B decreases monotonously. For $\tilde{T} > \tilde{T}_a$, the state is disordered with $\rho = 0$; And

at $\tilde{T} < \tilde{T}_a$, the state is ordered with $\rho > 0$. On the other hand, the physical temperature $T = JzB\tilde{T}$, and since B decreases with increasing with $\tilde{T}$, it is possible for T to decrease as $\tilde{T}$ increases. This is shown in fig. 2. This would mean for example that B would increase with increasing T, which is physically nonsensical. If the second order transition point $\tilde{T}_a$ belongs to such an unphysical $\tilde{T}$, it will not be accessible.

In ref.2, it was implicitly assumed that the mean field eqns. 9 and 10 have a two branch structure, so that at high T, $B = 0$ is the only solution, but below some T', a second solution with $B \neq 0$ appears. Instead, mean field eqns. actually have three branches of solutions for B or $\tilde{T}$ as functions of T. One is the trivial solution (upper branch), $B = 0$, or $\tilde{T} \to \infty$ at all T. The second branch solutions (lower branch) exist for all $T < T_t$, with $\tilde{T}$ monotomically increasing with T. For $T_g < T < T_t$, there is yet a third branch of solutions (middle branch), where $\tilde{T}$ goes to ∞ at $T = T_g$ and decreases as T increases until it merges and terminates with the second branch at $T = T_t$.

The solutions to the mean field equations correspond to extrema of the free energy. For $T < T_t$, there are more than one solutions, and the one giving the lowest free energy should be chosen. From the structure of the $\tilde{T}$ vs. T curve, we can deduce that as T is reduced, the free energy functional should behave as follows. For $T > T_t$, there is only one extremum, which is at $B = 0$. Between T_t and T_g, where there are three solutions, there is a local minimum at $B = 0$, a local maximum at $B = B_3$ (middle branch) and a secondary local minimum at $B = B_2$ (lower branch), with $B_2 > B_3$. As T decreases in the regime, B_3 moves towards 0 and at $T = T_g$, the curvature at $B = 0$ changes sign and becomes a local maximum below T_g, leaving B_2 as the only minimum. Given this, at some temperature T_b between T_g and T_t, the free energy at B_2 will become lower than at $B = 0$. Thus, at T_b, B will take a jump from 0 to a finite value of B_2. In Figs. 3-5, we show plots of free energy f vs. B to illustrate the above. In these plots, the $f(B)$ is calculated by solving eq. 10 for Λ with B as a variable and then evaluating f in eq. 7.

Thus, we see that in general, SBMFT gives a first order transition in B. Since B is a

measure of the short range order, the transition in B is fictitious and whether it is first order or continuous is not of any real significance. More importantly is where the Bose condensation transition occurs relative to this transition. Since in terms of $\widetilde{T}$, eq. 10 is just that for Bose-Einstein condensation, $\widetilde{T}_a \sim S^{2/d}$ for $d > 2$, as $S \to 0$, and hence so does the physical temperature T_a. Thus for small S, Bose condensation occurs at a temperature where the lowest branch is the stable solution, and the continuous transition at $\widetilde{T}_a$ accessible within SBMFT. As S increases, however, $\widetilde{T}_a$ continues to increase and for $S > S_c \simeq 0.15$, $\widetilde{T}_a > \widetilde{T}_b$, where the solution at the lower branch becomes meta-stable. At even larger S (e.g. $S = 1/2$), $\widetilde{T}_a$ becomes $> \widetilde{T}_t$, and the solution becomes unstable. Either way, for $S > S_c$, as the temperature increases from zero, the system undergoes a discontinuous transition at T_b from the LRO state with finite condensate density to the uncorrelated state with $B = 0$. There are two problems with this. The first is that result of a first order transition in magnetic long range order for the Heisenberg model in 3D is wrong. The second is that one of the major advantages of SBMFT is supposedly its applicability to both LRO and SRO state. But in fact, the stable solution is either completely uncorrelated or has LRO, just like standard Bethe-Weiss MFT.

III. ANTIFERROMAGNETIC HEISENBERG MODEL

In this section, we discuss the SBMFT for the AFM Heisenberg model described by the Hamiltonian,

$$H = J \sum_{<i,j>} S_i \cdot S_j, \tag{12}$$

where $J > 0$, and all other notations are the same as in the previous section for the FM case. We find that the same pathologies in the SBMFT solution for FM model are present also in the AFM model.

The hypercubic lattice is divided into two sub-lattices A and B. In a nearest neighbor pair $< ij >$, $i \in A$ and $j \in B$. As in the FM model, two Schwinger bosons $a_{i\sigma}$ with $\sigma = \pm 1$,

at each site i, and a bond field $A_{ij}^{\dagger} = \frac{1}{2}\sum_\sigma \sigma a_{i\sigma}^{\dagger}a_{j-\sigma}^{\dagger}$ are introduced. A_{ij} is anti-symmetric with respect to the interchange of i and j. A spin rotation by π about the y-axis is made at all the sites j on the sub-lattice B, so that $a_{j\uparrow}{\longrightarrow}a_{j\downarrow}$, $a_{j\downarrow}{\longrightarrow}a_{j\uparrow}$. The bond operator is then transformed as $A_{ij}^{\dagger} \longrightarrow A_{ij}^{\dagger} = \frac{1}{2}\sum_\sigma a_{i\sigma}^{\dagger}a_{j\sigma}^{\dagger}$. This canonical transformation preserves the constraint $\sum_\sigma a_{i\sigma}^{\dagger}a_{i\sigma} = 2S = 0, 1, 2, ...$

In terms of bosonic operators, the AFM Heisenberg model reads,

$$H = -\frac{J}{2}\sum_{<ij>}(A_{ij}^{\dagger}A_{ij} - 2S^2). \tag{13}$$

The mean field equations of the AFM model may be derived similarly to the FM model. A global Lagrangian multiplier λ to replace the constraint on every site, and a real and uniform mean field amplitude $< A_{ij} >=< A_{ij}^{\dagger} >= A$ are introduced. $A \neq 0$ describes short-range AFM correlations. After some algebra, the mean field Hamiltonian can be written as:

$$H_{MF} = E_0 + \lambda\sum_{k,\sigma}a_{k\sigma}^{\dagger}a_{k\sigma} - \frac{JAz}{2}\sum_{k,\sigma}\gamma_k(a_{k\sigma}^{\dagger}a_{-k\sigma}^{\dagger} + h.c), \tag{14}$$

with $\gamma_{\vec{k}} = \frac{1}{z}\sum_\delta e^{i\vec{k}.\vec{\delta}} = 1 - \epsilon_{\vec{k}}$, and $E_0 = \frac{1}{2}NzJS^2 - 2\lambda NS + JA^2Nz$.

H_{MF} is diagonalized by using the standard Bogoliubov transformation, yielding

$$H_{MF} = E_0 - \lambda N + \sum_k \omega_k(\alpha_k^{\dagger}\alpha_k + \beta_k^{\dagger}\beta_k + 1), \tag{15}$$

where $\omega_{\vec{k}} = (\lambda^2 - (JzA\gamma_{\vec{k}})^2)^{1/2}$. To find the optimal values of the mean fields, the free energy is differentiated with respect to A and λ, and the SBMFT equations for the AFM model are obtained,

$$S + \frac{1}{2} = \frac{1}{N}\sum_k \frac{\mu}{(\mu^2 - \gamma_k^2)^{1/2}}\Big(\frac{1}{e^{\tilde{\beta}(\mu^2-\gamma_k^2)^{1/2}} - 1} + \frac{1}{2}\Big), \tag{16}$$

$$A^2 = \frac{A}{N}\sum_k \frac{\gamma_k^2}{(\mu^2 - \gamma_k^2)^{1/2}}\Big(\frac{1}{e^{\tilde{\beta}(\mu^2-\gamma_k^2)^{1/2}} - 1} + \frac{1}{2}\Big), \tag{17}$$

where we have defined an effective inverse temperature $\tilde{\beta} = JAz\beta$ and an effective chemical potential $\mu = \frac{\lambda}{JAz}$. To describe the possible Schwinger boson condensed state,

condensation density ρ is introduced similar to that in the FM model, and the summations are replaced by integrals. The mean field eqns. become,

$$S + \frac{1}{2} = \rho + \int \frac{d^d\vec{k}}{(2\pi)^d} \frac{1}{(\mu^2 - \gamma_{\vec{k}}^2)^{1/2}} \Big(\frac{1}{e^{\tilde{\beta}(\mu^2 - \gamma_{\vec{k}}^2)^{1/2}} - 1} + \frac{1}{2} \Big), \qquad (18)$$

$$A^2 = A\Big(\rho + \int \frac{d^d\vec{k}}{(2\pi)^d} \frac{\gamma_{\vec{k}}^2}{(\mu^2 - \gamma_{\vec{k}}^2)^{1/2}} \Big(\frac{1}{e^{\tilde{\beta}(\mu^2 - \gamma_{\vec{k}}^2)^{1/2}} - 1} + \frac{1}{2} \Big)\Big). \qquad (19)$$

We now discuss the solutions of these eqns. Note that $\gamma_{\vec{k}}^2 \leq 1$, so we have $\mu \geq 1$. Similar to the FM case, $\rho = 0$ and $\mu > 1$ in the disordered phase, and $\rho > 0$ and $\mu = 1$ in the Schwinger boson condensation state, which corresponds to the Neel ordering phase of the spin system. The results are very similar to those for the 3D FM model.

The solutions for the mean field equations are smooth and monotonic functions of the effective temperature $\tilde{T}$, but not of the physical temperature T. In Fig. 6, we show the calculated $\tilde{T}$ as a function of T from the mean field eqns. for a typical spin $S = 1/2$. There are three branches of solutions in $\tilde{T}$. The $A = 0$ branch, and a middle and a lower branches. The Bose condensation point "a" (where $\mu = 1$ and $\rho = 0$) is again on the upper branch corresponding to a maximum in the free energy. We have calculated the free energy and found that the stable mean field solution jumps from a high T phase in the $A = 0$ branch to a low T phase in the lower branch with a finite condensation density at a temperature $T = T_b < T_a$. Therefore, the transition for LRO is first order. The qualitative feature of the free energy as a function of A is similar to those in Fig. 3-5 for the FM case. The critical spin for which $T_a = T_b$ for the AFM model is found to be $S_C \simeq 0.32$, larger than that in the FM model, but still substantially smaller than $1/2$. For $S > S_C$ the ordering transition within SBMFT is first order and for $S < S_C$, the transition is second order.

IV. CONCLUSIONS

We have re-examined the Schwinger boson MFT for quantum spin systems and found that for both the FM and AFM Heisenberg Hamiltonian, the mean field equations possess

in general three branches of solutions in the intermediate temperature regime. As a consequence, the system in 3D undergoes a first order transition from the ordered state to the completely uncorrelated state unless the spin S is very small. In addition to erroneously predicting a first order transition in magnetic ordering, there is no stable solution with finite SRO without LRO, the existence of which is supposed to be one of the advantages of SBMFT over Bethe-Weiss MFT or spin wave theory.

The three branch structure of the mean field solutions is not restricted to 3D. It is the origin of the reported discontinuous jump in the short-range MF amplitude A for the Heisenberg AFM on 2D square lattice as the temperature is increased [3]. For the 2D square lattice, however, the effective temperature for Bose condensation $\widetilde{T}_a = 0$, which means $\widetilde{T}_a < \widetilde{T}_b$ for all S. As a result, SBMFT is capable in that case of describing the SRO state at low temperature. It should not be assumed though that the pathologies associated with SBMFT reported in this paper is only relevant for $d > 2$. In fact, it will apply whenever the LRO state is destroyed by tuning some parameter if that parameter is sufficiently large. One example of this is the bilayered Heisenberg AFM Hamiltonian in 2D, which received interest a few years ago due to its relevance to YBCO [6–8]. In the bilayered system, the in-plane AF magnetic LRO is destroyed by sufficiently large inter-layer coupling which favors having inter-plane neighbors forming singlets [5,6,9–16]. Using SBMFT, Ng et al [5] found for $S > S_c \simeq 0.35$, the transition is first order from finite condensate density to the state of disconnected inter-plane singlets with zero in-plane correlations. This result contradicted the hypothesis that the 2D bilayered AFM at $T = 0$ is in the same universality class as the 3D non-linear sigma model at finite T, a hypothesis partially confirmed by finite sized numerical calculations for $S = 1/2$ [14]. One possibility is that SBMFT is qualitatively correct, but that the value of S_c calculated is too small. Subsequently, Gelfand et al [17] provided further evidence that the transition for arbitrary S is continuous and that the SBMFT prediction of first order transition is incorrect. However, it was not clear why SBMFT gave such a qualitatively incorrect result. From the present work, we can now understand that the first order transition reported there is an artifact of the same pathologies of the SBMFT reported

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in this paper.

Finally, while we have focused on SU(2) Heisenberg Hamiltonian in this paper, the results are a consequence of the structure of the mean field equations, and therefore will be valid for SU(N) generalization of the Heisenberg Hamiltonian for which the SBMFT approach above [1] can be applied.

V. ACKNOWLEDGMENTS

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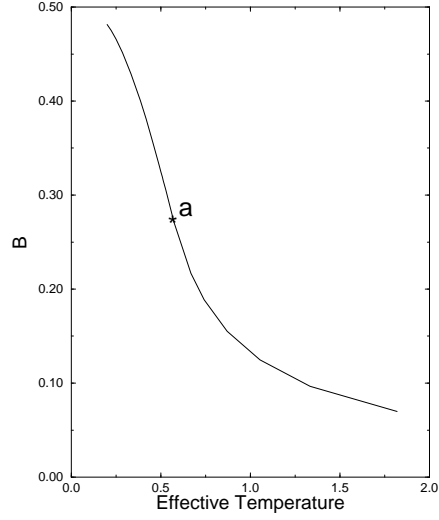[17] M. P. Gelfand, W.H. Zheng, C.J. Hamer and J. Oitmaa, Phys. Rev. B 57, 392 (1998)

FIG. 1. Effective temperature $(\tilde{T})$ dependance of B for three dimensional spin 1/2 Heisenberg ferromagnetic Hamiltonian. Bose condensation occurs at $\tilde{T}_a$.
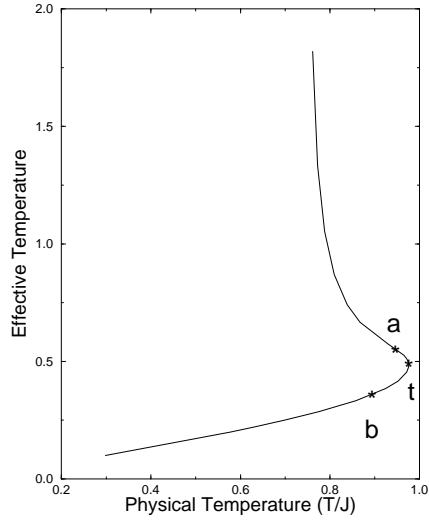

FIG. 2. Effective temperature $(\tilde{T})$ as a function of physical temperature (T/J) for three dimensional spin 1/2 Heisenberg ferromagnetic Hamiltonian.
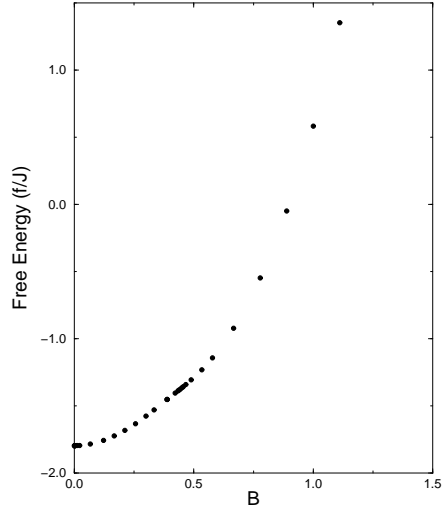
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FIG. 3.   SB mean field free energy at $T = 1.3333J > T_t$ for three dimensional spin $1/2$ Heisenberg ferromagnetic Hamiltonian.
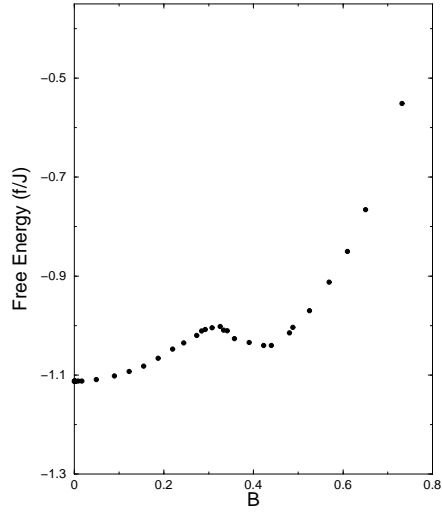

FIG. 4. SB mean field free energy at $T_b < T = 0.9753J < T_t$ for three dimensional spin $1/2$ Heisenberg ferromagnetic Hamiltonian.
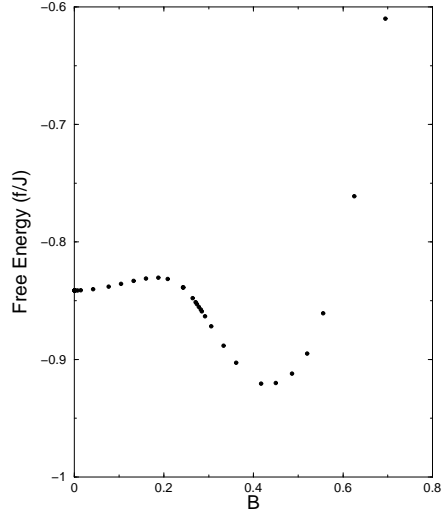
FIG. 5. SB mean field free energy at $T = 0.8333J < T_b$ for three dimensional spin 1/2 Heisenberg ferromagnetic Hamiltonian.
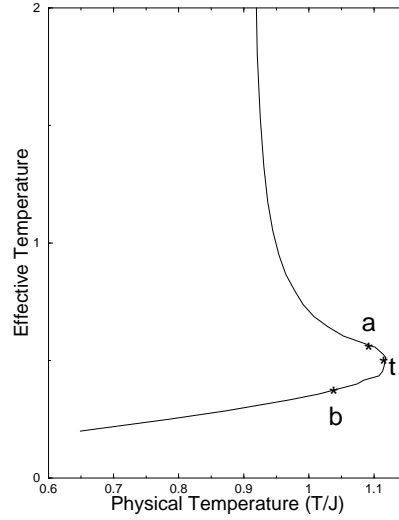

FIG. 6. Effective temperature ($\tilde{T}$) as a function of physical temperature (T/J) for three dimensional spin 1/2 Heisenberg antiferromagnetic Hamiltonian.